Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U7F
Title	:	Crystal Structure of the phosphorylated Smad3/Smad4 heterotrimeric complex
Authors	:	Chacko, B.M.; Qin, B.Y.; Tiwari, A.; Shi, G.; Lam, S.; Hayward, L.J.; de Caestecker, M.; Lin, K.
Deposited on	:	2004-08-03
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

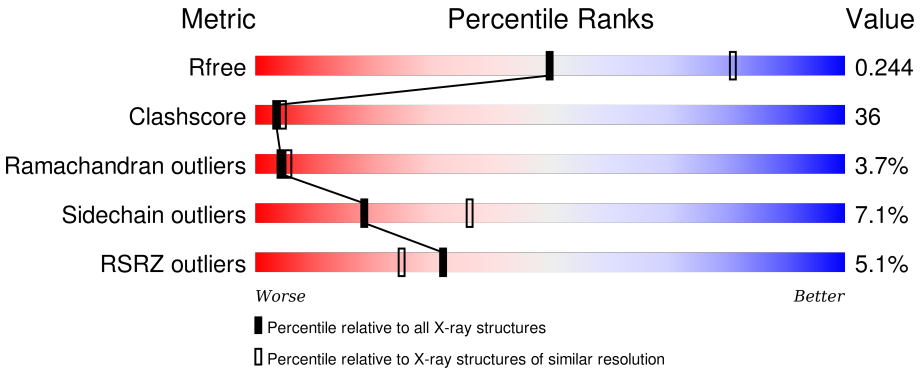
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	198	2% 53% 40% 7%
1	C	198	5% 50% 40% 8%
2	B	239	8% 36% 39% 5% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4983 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mothers against decapentaplegic homolog 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	P	S	0	0	0
			1571	986	277	293	2	13			
1	C	196	Total	C	N	O	P	S	0	0	0
			1556	976	275	290	2	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	SEP	SER	MODIFIED RESIDUE	UNP P84022
A	425	SEP	SER	MODIFIED RESIDUE	UNP P84022
C	423	SEP	SER	MODIFIED RESIDUE	UNP P84022
C	425	SEP	SER	MODIFIED RESIDUE	UNP P84022

- Molecule 2 is a protein called Mothers against decapentaplegic homolog 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	7	0
			1601	1015	285	289	12			

- Molecule 3 is water.

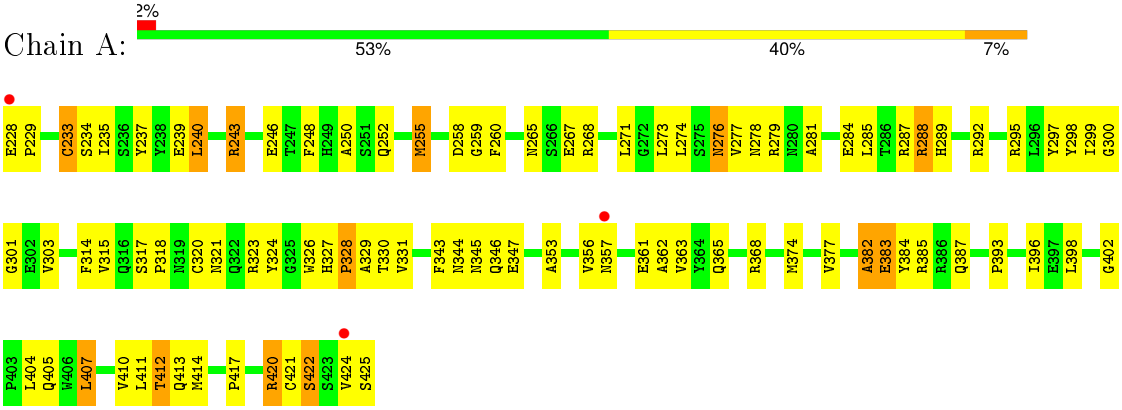
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	63	Total	O	0	0
			63	63		
3	C	97	Total	O	0	0
			97	97		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

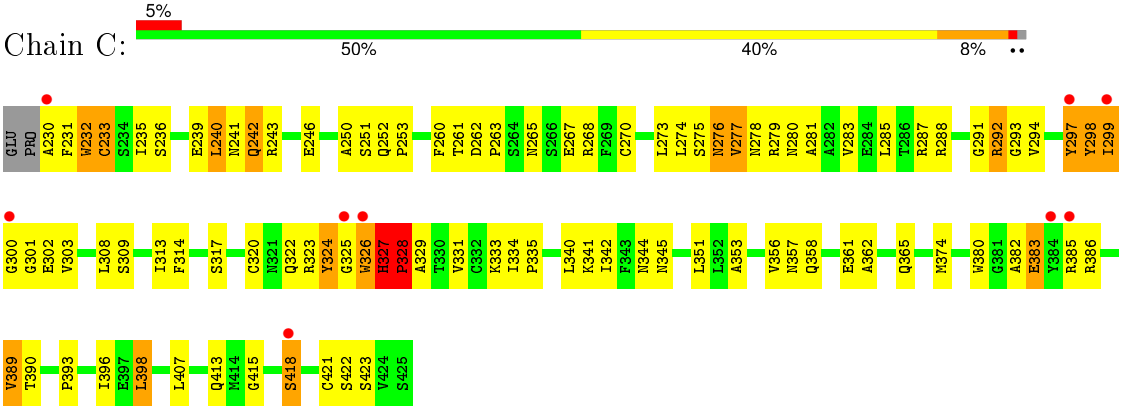
• Molecule 1: Mothers against decapentaplegic homolog 3

Chain A:



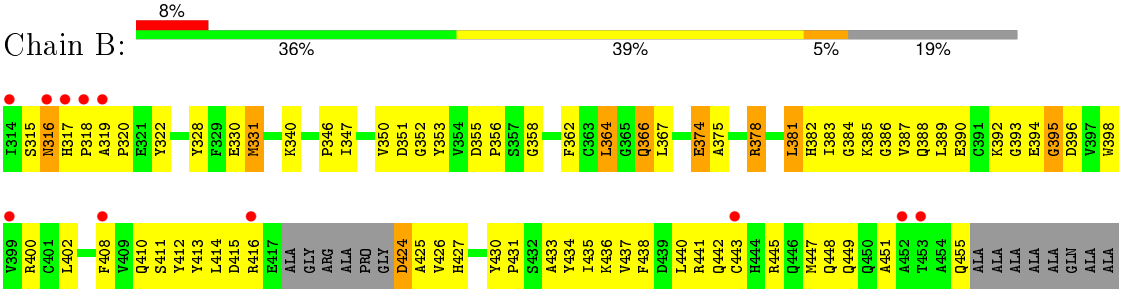
• Molecule 1: Mothers against decapentaplegic homolog 3

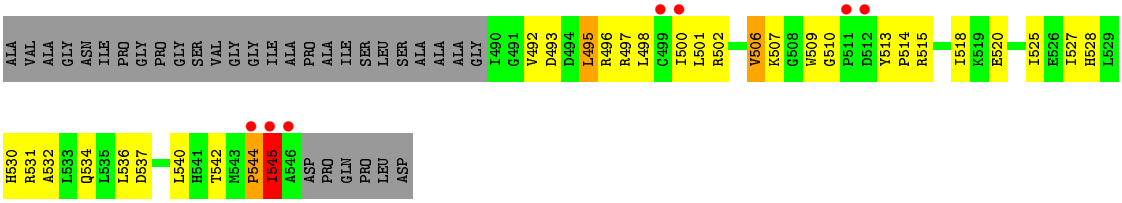
Chain C:



• Molecule 2: Mothers against decapentaplegic homolog 4

Chain B:




ALA VAL ALA GLY ASN ILE PRO GLY PRO GLY SER VAL GLY GLY ILE ALA PRO ALA ILE SER LEU SER ALA ALA ALA GLY I490 G491 V492 D493 D494 L495 R496 R497 L498 C499 I500 L501 R502 V506 K507 G508 W509 G510 P511 D512 Y513 P514 R515 I518 K519 E520 I525 E526 I527 H528 L529
H530 R531 A532 L533 Q534 L535 L536 D537 L540 H541 T542 M543 P544 T545 A546 ASP PRO GLN PRO LEU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.47Å 60.55Å 205.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 30.48 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.4 (100.00-2.60) 92.0 (30.48-2.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.247 0.231 , 0.244	Depositor DCC
R_{free} test set	886 reflections (4.83%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 21132 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/1590	0.70	0/2159
1	C	0.41	0/1573	0.77	4/2135 (0.2%)
2	B	0.37	0/1642	0.67	0/2228
All	All	0.41	0/4805	0.72	4/6522 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	326	TRP	N-CA-C	6.20	127.74	111.00
1	C	386	ARG	N-CA-C	-6.16	94.36	111.00
1	C	325	GLY	N-CA-C	5.99	128.06	113.10
1	C	326	TRP	CA-CB-CG	-5.87	102.55	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1506	110	0
1	C	1556	0	1494	109	0
2	B	1601	0	1558	137	0
3	A	95	0	0	35	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	63	0	0	25	0
3	C	97	0	0	23	1
All	All	4983	0	4558	336	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:CE1	1:C:299:ILE:HG12	1.87	1.10
2:B:318[A]:PRO:HB2	2:B:531:ARG:NH1	1.75	1.02
2:B:318[A]:PRO:HB2	2:B:531:ARG:HH12	1.26	0.99
1:C:273:LEU:HD11	3:C:470:HOH:O	1.63	0.99
1:C:242:GLN:HG3	3:C:512:HOH:O	1.63	0.98
2:B:319[A]:ALA:H	2:B:531:ARG:HH12	0.96	0.95
2:B:315[A]:SER:O	2:B:316[A]:ASN:HB2	1.64	0.94
2:B:425:ALA:HB2	3:B:126:HOH:O	1.68	0.94
1:C:418:SER:HB3	3:C:509:HOH:O	1.67	0.93
2:B:319[A]:ALA:H	2:B:531:ARG:NH1	1.67	0.91
2:B:426:VAL:HG21	3:B:45:HOH:O	1.70	0.90
1:A:229:PRO:HG3	3:A:489:HOH:O	1.71	0.89
2:B:319[A]:ALA:HB2	3:B:198:HOH:O	1.72	0.89
1:A:315:VAL:HG22	1:A:374:MET:HG2	1.56	0.88
1:A:361:GLU:HG3	1:A:362:ALA:H	1.37	0.87
2:B:366:GLN:NE2	3:B:77:HOH:O	2.07	0.87
1:C:327:HIS:O	1:C:329:ALA:N	2.06	0.87
1:C:382:ALA:O	1:C:383:GLU:HB2	1.74	0.86
1:C:252:GLN:HG3	1:C:267:GLU:HG2	1.58	0.86
1:A:229:PRO:HD3	3:A:455:HOH:O	1.75	0.85
1:A:382:ALA:C	1:A:383:GLU:HG2	1.93	0.85
2:B:495:LEU:HD21	2:B:536:LEU:HD11	1.59	0.84
2:B:424:ASP:N	3:B:98:HOH:O	2.10	0.84
2:B:426:VAL:HG21	3:B:170:HOH:O	1.78	0.83
2:B:497:ARG:NH1	3:B:120:HOH:O	2.10	0.83
1:C:333:LYS:HE2	1:C:335:PRO:HG3	1.61	0.83
1:C:297:TYR:HE1	1:C:299:ILE:HG12	1.39	0.81
1:C:260:PHE:O	1:C:270:CYS:HB3	1.80	0.80
2:B:520:GLU:HB2	3:B:169:HOH:O	1.81	0.80
1:A:365:GLN:HE21	1:A:368:ARG:NH2	1.80	0.79
1:A:365:GLN:HB3	1:A:368:ARG:NH2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:LEU:HD23	3:C:468:HOH:O	1.84	0.77
1:A:300:GLY:HA3	3:A:460:HOH:O	1.83	0.77
2:B:319[A]:ALA:CB	3:B:198:HOH:O	2.30	0.77
1:C:324:TYR:HB3	3:C:456:HOH:O	1.85	0.76
2:B:426:VAL:HG11	2:B:510:GLY:HA3	1.68	0.75
1:C:273:LEU:HD21	3:C:470:HOH:O	1.87	0.75
1:A:318:PRO:HG3	3:A:509:HOH:O	1.87	0.75
1:C:231:PHE:O	1:C:233:CYS:N	2.18	0.74
2:B:319[A]:ALA:N	2:B:531:ARG:HH12	1.80	0.74
2:B:506:VAL:HG21	3:B:64:HOH:O	1.88	0.74
1:A:243:ARG:NH2	3:A:497:HOH:O	2.21	0.73
3:B:42:HOH:O	1:C:246:GLU:HG2	1.89	0.73
1:C:292:ARG:HB2	1:C:308:LEU:HB3	1.70	0.73
1:A:424:VAL:HG23	2:B:514:PRO:HG2	1.70	0.72
2:B:426:VAL:CG2	3:B:170:HOH:O	2.36	0.72
2:B:537:ASP:OD2	1:C:260:PHE:HB3	1.88	0.72
1:C:358:GLN:HB2	1:C:362:ALA:CB	2.19	0.72
2:B:520:GLU:OE2	3:B:169:HOH:O	2.07	0.72
1:A:346:GLN:OE1	3:A:476:HOH:O	2.07	0.72
1:A:265:ASN:HB3	3:A:463:HOH:O	1.90	0.72
1:A:301:GLY:N	3:A:460:HOH:O	2.17	0.71
1:C:277:VAL:HG23	1:C:278:ASN:ND2	2.06	0.71
1:C:235:ILE:HG22	1:C:396:ILE:HG12	1.72	0.71
2:B:346:PRO:O	2:B:390:GLU:HA	1.90	0.71
2:B:448:GLN:HG2	3:B:105:HOH:O	1.91	0.71
1:A:382:ALA:O	1:A:383:GLU:HG2	1.91	0.70
1:A:410:VAL:O	1:A:414:MET:HG2	1.91	0.70
2:B:496:ARG:HH22	1:C:275:SER:CB	2.05	0.70
1:C:415:GLY:O	3:C:478:HOH:O	2.09	0.70
1:C:298:TYR:O	3:C:486:HOH:O	2.10	0.70
1:C:262:ASP:O	3:C:516:HOH:O	2.09	0.69
2:B:347:ILE:HG13	2:B:390:GLU:HG3	1.73	0.69
1:C:236:SER:OG	3:C:513:HOH:O	2.11	0.69
1:A:365:GLN:HE21	1:A:368:ARG:HH22	1.40	0.69
1:C:274:LEU:HA	3:C:468:HOH:O	1.93	0.69
1:C:301:GLY:CA	1:C:345:ASN:HD22	2.05	0.69
2:B:451:ALA:O	2:B:455:GLN:HG3	1.93	0.69
2:B:378:ARG:O	2:B:381:LEU:HB2	1.93	0.69
2:B:318[A]:PRO:HB2	2:B:531:ARG:CZ	2.22	0.68
2:B:374:GLU:CD	2:B:374:GLU:H	1.97	0.68
2:B:346:PRO:HG2	2:B:347:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:VAL:O	3:B:67:HOH:O	2.12	0.68
1:C:275:SER:N	3:C:458:HOH:O	1.96	0.68
1:A:259:GLY:HA3	3:A:492:HOH:O	1.92	0.67
1:C:317:SER:HB3	1:C:320:CYS:HB3	1.77	0.67
2:B:506:VAL:CG2	3:B:64:HOH:O	2.41	0.67
1:C:326:TRP:HA	1:C:326:TRP:CE3	2.30	0.66
2:B:398:TRP:CZ2	2:B:436:LYS:HB2	2.30	0.66
2:B:350:VAL:HG13	2:B:364:LEU:HD11	1.75	0.66
1:A:420:ARG:HG3	1:A:421:CYS:H	1.59	0.66
2:B:425:ALA:CB	3:B:126:HOH:O	2.35	0.66
2:B:496:ARG:HH22	1:C:275:SER:HB2	1.60	0.66
2:B:544:PRO:O	2:B:545:ILE:O	2.14	0.66
2:B:412:TYR:HA	2:B:415:ASP:OD2	1.96	0.66
1:A:317:SER:HB3	1:A:320:CYS:HB3	1.77	0.65
2:B:392:LYS:HD2	2:B:398:TRP:NE1	2.09	0.65
2:B:433:ALA:HB1	2:B:435:ILE:CD1	2.27	0.65
2:B:435:ILE:N	2:B:435:ILE:HD12	2.11	0.65
2:B:392:LYS:HD2	2:B:398:TRP:CD1	2.32	0.64
2:B:544:PRO:C	2:B:545:ILE:HD12	2.17	0.64
1:C:283:VAL:O	1:C:287:ARG:HG3	1.98	0.64
1:A:328:PRO:O	3:A:509:HOH:O	2.14	0.64
2:B:378:ARG:HH11	2:B:378:ARG:CB	2.11	0.64
1:C:393:PRO:HD2	3:C:460:HOH:O	1.97	0.64
2:B:400:ARG:HG2	2:B:402:LEU:CD1	2.27	0.64
2:B:317[A]:HIS:HB3	2:B:318[A]:PRO:HA	1.79	0.64
1:A:278:ASN:HD21	1:C:241:ASN:HD22	1.43	0.64
1:A:235:ILE:HD11	1:A:255:MET:HE1	1.79	0.63
2:B:495:LEU:HD23	2:B:496:ARG:N	2.13	0.63
1:A:321:ASN:ND2	1:A:330:THR:HB	2.13	0.63
1:A:356:VAL:HG23	1:A:357:ASN:ND2	2.14	0.63
1:C:380:TRP:CZ2	1:C:389:VAL:HG13	2.34	0.63
1:C:334:ILE:HD11	1:C:340:LEU:HD22	1.81	0.63
2:B:493:ASP:OD1	1:C:287:ARG:NH1	2.33	0.62
1:C:280:ASN:OD1	1:C:281:ALA:N	2.33	0.62
1:A:235:ILE:HD11	1:A:255:MET:CE	2.29	0.62
1:C:239:GLU:O	1:C:240:LEU:HB2	2.00	0.62
1:A:279:ARG:HA	3:A:462:HOH:O	2.00	0.61
2:B:425:ALA:O	2:B:426:VAL:HG22	2.00	0.61
1:A:234:SER:HB3	3:A:475:HOH:O	2.00	0.61
1:C:380:TRP:CE2	1:C:389:VAL:HG13	2.36	0.61
1:C:273:LEU:C	1:C:273:LEU:HD12	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ARG:NH2	1:C:275:SER:HA	2.15	0.61
2:B:441:ARG:HG2	3:B:188:HOH:O	2.01	0.61
1:C:235:ILE:HG22	1:C:396:ILE:CG1	2.31	0.60
1:C:331:VAL:HG21	1:C:380:TRP:O	2.01	0.60
2:B:385:LYS:HB2	2:B:402:LEU:O	2.01	0.60
1:A:361:GLU:HG3	1:A:362:ALA:N	2.12	0.60
1:A:328:PRO:HA	3:A:502:HOH:O	2.01	0.60
2:B:433:ALA:HB1	2:B:435:ILE:HD11	1.83	0.60
2:B:393:GLY:C	2:B:395:GLY:H	2.04	0.60
1:A:387:GLN:HG3	3:A:480:HOH:O	2.02	0.60
1:A:233:CYS:C	3:A:475:HOH:O	2.39	0.60
2:B:330:GLU:O	2:B:331:MET:HB2	2.01	0.60
2:B:393:GLY:O	2:B:395:GLY:N	2.34	0.59
1:C:276:ASN:HD22	1:C:276:ASN:C	2.06	0.59
1:C:322:GLN:HE22	1:C:351:LEU:HD22	1.67	0.59
1:A:365:GLN:NE2	1:A:368:ARG:NH2	2.52	0.58
1:A:271:LEU:O	1:A:287:ARG:NH2	2.36	0.58
2:B:426:VAL:O	2:B:426:VAL:HG23	2.03	0.58
2:B:542:THR:C	2:B:544:PRO:HD3	2.24	0.58
1:C:235:ILE:CG2	1:C:396:ILE:HG12	2.33	0.58
1:A:382:ALA:O	1:A:383:GLU:CG	2.51	0.58
1:A:353:ALA:O	1:A:356:VAL:HG22	2.03	0.58
2:B:315[A]:SER:O	2:B:316[A]:ASN:CB	2.46	0.58
2:B:319[A]:ALA:N	2:B:531:ARG:NH1	2.47	0.58
2:B:447:MET:HE1	2:B:532:ALA:O	2.03	0.57
1:A:412:THR:HA	2:B:353:TYR:CE2	2.38	0.57
1:C:302:GLU:OE2	1:C:341:LYS:HD3	2.04	0.57
1:A:250:ALA:HB2	1:A:255:MET:HE1	1.86	0.57
1:C:297:TYR:CZ	1:C:299:ILE:HG12	2.38	0.57
1:C:252:GLN:HG3	1:C:267:GLU:CG	2.32	0.57
2:B:536:LEU:O	2:B:540:LEU:HG	2.05	0.57
1:A:297:TYR:O	1:A:303:VAL:HA	2.05	0.57
1:C:358:GLN:HB2	1:C:362:ALA:HB3	1.86	0.57
1:A:252:GLN:HG3	1:A:267:GLU:HG2	1.86	0.56
1:C:357:ASN:HB2	3:C:517:HOH:O	2.05	0.56
2:B:493:ASP:OD2	1:C:287:ARG:HD3	2.06	0.56
1:A:424:VAL:HG23	2:B:514:PRO:CG	2.34	0.56
2:B:500:ILE:HD11	2:B:528:HIS:NE2	2.21	0.56
2:B:545:ILE:HD12	2:B:545:ILE:N	2.21	0.56
1:C:292:ARG:HH11	1:C:292:ARG:HG2	1.72	0.55
1:A:343:PHE:HE2	1:A:345:ASN:OD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:VAL:HG22	2:B:362:PHE:HB3	1.88	0.55
1:C:265:ASN:HB3	1:C:268:ARG:HB2	1.88	0.55
1:C:299:ILE:CG2	3:C:454:HOH:O	2.55	0.55
1:A:385:ARG:N	3:A:479:HOH:O	2.30	0.55
1:C:299:ILE:O	1:C:299:ILE:HG22	2.07	0.54
1:C:353:ALA:O	1:C:356:VAL:HG22	2.07	0.54
2:B:410:GLN:NE2	3:B:88:HOH:O	2.40	0.53
2:B:536:LEU:HD12	2:B:536:LEU:O	2.08	0.53
1:C:303:VAL:HG12	1:C:342:ILE:HD11	1.91	0.52
2:B:322:TYR:HB2	2:B:530:HIS:CE1	2.44	0.52
2:B:387:VAL:HG23	2:B:388:GLN:N	2.24	0.52
1:C:313:ILE:HG13	1:C:313:ILE:O	2.08	0.52
1:C:273:LEU:O	3:C:468:HOH:O	2.19	0.52
2:B:320[A]:PRO:HB2	2:B:322:TYR:O	2.10	0.52
2:B:411:SER:HB3	2:B:414:LEU:HD12	1.92	0.52
1:C:252:GLN:CG	1:C:267:GLU:HG2	2.34	0.52
1:A:273:LEU:HD12	1:A:274:LEU:N	2.25	0.52
2:B:398:TRP:CH2	2:B:436:LYS:HB2	2.45	0.51
2:B:317[B]:HIS:HB2	2:B:318[B]:PRO:HD2	1.92	0.51
2:B:364:LEU:N	2:B:364:LEU:CD1	2.73	0.51
1:C:423:SEP:P	3:C:452:HOH:O	2.69	0.51
1:A:421:CYS:SG	2:B:507:LYS:NZ	2.84	0.50
1:A:417:PRO:HB2	2:B:382:HIS:HE1	1.76	0.50
2:B:493:ASP:C	3:B:120:HOH:O	2.49	0.50
1:A:421:CYS:HB2	2:B:382:HIS:CD2	2.46	0.50
2:B:340:LYS:HD3	3:B:121:HOH:O	2.12	0.50
1:A:259:GLY:CA	3:A:492:HOH:O	2.57	0.50
1:A:411:LEU:C	1:A:413:GLN:H	2.15	0.50
2:B:492:VAL:HA	2:B:495:LEU:HD22	1.94	0.50
2:B:435:ILE:HG22	2:B:436:LYS:N	2.27	0.50
2:B:412:TYR:CE2	2:B:498:LEU:HD23	2.47	0.50
1:A:239:GLU:O	1:A:240:LEU:HB2	2.11	0.50
1:A:324:TYR:HD1	1:A:326:TRP:CH2	2.30	0.49
1:A:326:TRP:O	1:A:327:HIS:C	2.50	0.49
1:C:243:ARG:HG2	1:C:243:ARG:HH11	1.75	0.49
2:B:495:LEU:HD11	2:B:536:LEU:CD1	2.42	0.49
2:B:398:TRP:CE2	2:B:436:LYS:HB2	2.47	0.49
2:B:315[B]:SER:HG	2:B:317[B]:HIS:CD2	2.30	0.49
2:B:414:LEU:HD11	2:B:437:VAL:HG12	1.93	0.49
1:A:229:PRO:CD	3:A:455:HOH:O	2.45	0.49
1:A:420:ARG:CG	1:A:421:CYS:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:HB2	1:A:268:ARG:NH2	2.28	0.49
1:A:384:TYR:O	1:A:387:GLN:NE2	2.45	0.49
2:B:495:LEU:HD21	2:B:536:LEU:HD21	1.94	0.48
1:A:268:ARG:HB2	3:A:463:HOH:O	2.13	0.48
1:C:314:PHE:CD1	1:C:314:PHE:N	2.81	0.48
2:B:318[A]:PRO:HB2	2:B:531:ARG:NH2	2.29	0.48
1:C:241:ASN:HB3	1:C:390:THR:HB	1.96	0.48
2:B:375:ALA:HA	2:B:378:ARG:NH1	2.28	0.48
2:B:509:TRP:O	2:B:513:TYR:HD2	1.96	0.48
1:C:413:GLN:HA	1:C:413:GLN:NE2	2.28	0.47
2:B:328:TYR:HA	2:B:525:ILE:HG22	1.96	0.47
2:B:352:GLY:HA3	2:B:383:ILE:HB	1.96	0.47
1:A:356:VAL:HG23	1:A:357:ASN:HD22	1.79	0.47
2:B:384:GLY:C	2:B:386:GLY:H	2.17	0.47
1:C:230:ALA:N	3:C:472:HOH:O	2.47	0.47
2:B:434:TYR:C	2:B:435:ILE:HD12	2.35	0.47
1:A:314:PHE:HB3	1:A:331:VAL:CG1	2.45	0.47
1:C:326:TRP:HE3	1:C:327:HIS:H	1.62	0.47
1:A:365:GLN:NE2	1:A:368:ARG:HH22	2.07	0.47
1:A:250:ALA:HB2	1:A:255:MET:CE	2.45	0.47
1:C:279:ARG:NH2	1:C:287:ARG:NH2	2.63	0.47
1:C:231:PHE:CE1	1:C:251:SER:HB3	2.50	0.47
2:B:435:ILE:CG2	2:B:436:LYS:N	2.77	0.47
2:B:441:ARG:HD2	3:B:222:HOH:O	2.14	0.47
1:A:326:TRP:HB3	1:A:330:THR:OG1	2.15	0.47
1:C:276:ASN:ND2	1:C:276:ASN:C	2.67	0.47
1:A:405:GLN:NE2	3:A:489:HOH:O	2.49	0.46
2:B:495:LEU:HD11	2:B:536:LEU:HD11	1.97	0.46
2:B:350:VAL:HG13	2:B:364:LEU:CD1	2.45	0.46
1:A:421:CYS:O	1:A:422:SER:O	2.33	0.46
2:B:435:ILE:CD1	2:B:435:ILE:N	2.78	0.46
2:B:495:LEU:C	2:B:495:LEU:HD23	2.36	0.46
2:B:378:ARG:HB2	2:B:378:ARG:HH11	1.78	0.46
1:C:231:PHE:O	1:C:250:ALA:O	2.34	0.46
1:A:363:VAL:HG12	1:A:407:LEU:HD21	1.98	0.46
2:B:440:LEU:O	2:B:443:CYS:HB3	2.15	0.46
1:A:402:GLY:HA2	3:A:455:HOH:O	2.15	0.46
1:C:231:PHE:C	1:C:233:CYS:H	2.14	0.46
2:B:500:ILE:CG2	2:B:501:LEU:N	2.78	0.46
1:C:273:LEU:C	1:C:273:LEU:CD1	2.84	0.46
1:C:361:GLU:O	1:C:365:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:HIS:O	1:A:329:ALA:N	2.49	0.45
1:C:294:VAL:HG21	1:C:374:MET:HE1	1.98	0.45
2:B:319[B]:ALA:HA	2:B:531:ARG:NH1	2.31	0.45
1:C:277:VAL:C	1:C:278:ASN:HD22	2.20	0.45
1:A:289:HIS:CE1	1:C:421:CYS:HB2	2.50	0.45
1:C:327:HIS:HA	1:C:328:PRO:HD2	1.68	0.45
2:B:515:ARG:HB3	2:B:520:GLU:HB3	1.98	0.45
1:A:417:PRO:HB2	2:B:382:HIS:CE1	2.51	0.45
2:B:389:LEU:HD13	2:B:527:ILE:HD13	1.98	0.45
1:A:404:LEU:HB3	2:B:356:PRO:HD3	1.97	0.45
1:C:274:LEU:O	1:C:287:ARG:NH2	2.49	0.45
2:B:425:ALA:O	2:B:426:VAL:CG2	2.65	0.45
1:A:292:ARG:O	3:A:459:HOH:O	2.21	0.45
1:A:317:SER:HB3	1:A:320:CYS:CB	2.44	0.45
1:C:323:ARG:HH12	1:C:341:LYS:HB3	1.81	0.45
1:C:285:LEU:HD12	1:C:288:ARG:HH21	1.82	0.45
1:A:237:TYR:CG	1:A:271:LEU:HD22	2.52	0.45
2:B:320[B]:PRO:HD3	2:B:534:GLN:OE1	2.17	0.45
1:C:299:ILE:HA	1:C:299:ILE:HD13	1.84	0.45
2:B:438:PHE:HA	3:B:67:HOH:O	2.17	0.45
2:B:393:GLY:C	2:B:395:GLY:N	2.71	0.45
1:C:291:GLY:C	1:C:293:GLY:H	2.18	0.44
1:A:405:GLN:HG3	2:B:355:ASP:OD2	2.17	0.44
2:B:317[A]:HIS:HA	2:B:318[A]:PRO:O	2.17	0.44
1:C:252:GLN:HA	1:C:253:PRO:HD3	1.87	0.44
1:A:324:TYR:HD1	1:A:326:TRP:CZ3	2.36	0.44
2:B:515:ARG:HH11	2:B:515:ARG:HG2	1.83	0.44
1:C:334:ILE:HD11	1:C:340:LEU:CD2	2.46	0.44
1:A:288:ARG:NH1	1:C:361:GLU:OE2	2.51	0.44
1:A:420:ARG:HG3	1:A:421:CYS:N	2.27	0.44
2:B:351:ASP:CG	2:B:353:TYR:HD1	2.22	0.44
2:B:408:PHE:CD1	2:B:408:PHE:N	2.87	0.43
1:A:344:ASN:OD1	1:A:347:GLU:HG3	2.18	0.43
1:A:277:VAL:HG22	3:A:432:HOH:O	2.18	0.43
2:B:425:ALA:C	2:B:426:VAL:HG22	2.38	0.43
2:B:495:LEU:HD21	2:B:536:LEU:CD1	2.39	0.43
1:A:425:SEP:OG	1:A:425:SEP:O	2.36	0.43
1:A:229:PRO:CG	3:A:489:HOH:O	2.47	0.43
1:A:328:PRO:HB3	3:A:509:HOH:O	2.18	0.43
1:C:273:LEU:CD1	3:C:470:HOH:O	2.43	0.43
1:C:232:TRP:O	1:C:233:CYS:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH1	1:C:361:GLU:OE1	2.51	0.43
1:C:279:ARG:NH2	1:C:287:ARG:CZ	2.82	0.43
1:A:361:GLU:CG	1:A:362:ALA:H	2.21	0.43
2:B:412:TYR:CD2	2:B:498:LEU:HD23	2.54	0.42
1:A:321:ASN:HB2	3:A:502:HOH:O	2.19	0.42
1:C:291:GLY:O	1:C:293:GLY:N	2.52	0.42
1:A:228:GLU:HA	1:A:229:PRO:HD3	1.75	0.42
1:A:246:GLU:HG2	3:C:496:HOH:O	2.19	0.42
1:C:309:SER:CB	3:C:474:HOH:O	2.67	0.42
2:B:509:TRP:CG	2:B:510:GLY:N	2.86	0.42
1:A:324:TYR:CD1	1:A:326:TRP:CH2	3.07	0.42
1:C:334:ILE:CD1	1:C:340:LEU:HD22	2.48	0.42
1:A:411:LEU:O	1:A:413:GLN:N	2.53	0.42
1:A:299:ILE:HD11	3:A:451:HOH:O	2.19	0.42
1:C:261:THR:O	1:C:263:PRO:HD3	2.20	0.42
1:C:235:ILE:HG22	1:C:396:ILE:CD1	2.49	0.42
1:A:314:PHE:O	1:A:374:MET:HA	2.19	0.41
1:A:318:PRO:CB	3:A:509:HOH:O	2.68	0.41
1:C:292:ARG:CG	1:C:292:ARG:HH11	2.33	0.41
1:C:235:ILE:HG23	1:C:398:LEU:HD12	2.02	0.41
1:A:377:VAL:O	3:A:458:HOH:O	2.21	0.41
1:C:231:PHE:HE1	1:C:251:SER:HB3	1.85	0.41
2:B:400:ARG:HA	2:B:433:ALA:O	2.20	0.41
1:C:331:VAL:HG23	1:C:331:VAL:O	2.19	0.41
1:A:276:ASN:HB3	1:A:279:ARG:HB2	2.01	0.41
1:A:295:ARG:HD3	1:A:297:TYR:CZ	2.55	0.41
1:A:411:LEU:C	1:A:413:GLN:N	2.73	0.41
2:B:320[B]:PRO:HB2	2:B:322:TYR:O	2.20	0.41
2:B:530:HIS:O	2:B:534:GLN:HG3	2.21	0.41
1:A:239:GLU:HA	1:A:393:PRO:O	2.20	0.41
1:A:281:ALA:O	1:A:285:LEU:HB2	2.20	0.41
1:A:298:TYR:CE1	3:A:500:HOH:O	2.72	0.41
1:A:234:SER:HA	1:A:248:PHE:O	2.21	0.41
1:A:383:GLU:HA	3:A:452:HOH:O	2.19	0.41
1:A:321:ASN:HD22	1:A:330:THR:H	1.69	0.41
1:C:292:ARG:CD	3:C:503:HOH:O	2.68	0.41
1:A:387:GLN:CG	3:A:480:HOH:O	2.66	0.41
2:B:330:GLU:O	2:B:331:MET:CB	2.69	0.41
1:C:302:GLU:HG2	1:C:344:ASN:HD22	1.86	0.41
2:B:328:TYR:CD2	2:B:367:LEU:HD12	2.56	0.41
1:C:292:ARG:HD2	3:C:503:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:CG1	1:A:407:LEU:HD21	2.51	0.41
2:B:496:ARG:NH2	1:C:275:SER:CA	2.83	0.40
1:A:258:ASP:HB3	3:A:459:HOH:O	2.19	0.40
1:A:398:LEU:N	1:A:398:LEU:HD12	2.37	0.40
2:B:413:TYR:HE1	2:B:442:GLN:NE2	2.19	0.40
1:A:314:PHE:CD1	1:A:314:PHE:N	2.89	0.40
1:C:301:GLY:HA3	1:C:345:ASN:HD22	1.83	0.40
1:C:243:ARG:HG2	1:C:243:ARG:NH1	2.37	0.40
2:B:502:ARG:HB3	2:B:518:ILE:HD13	2.04	0.40
1:A:284:GLU:OE2	3:A:466:HOH:O	2.22	0.40
1:C:299:ILE:O	1:C:300:GLY:C	2.60	0.40
1:A:323:ARG:HD2	1:A:324:TYR:CE2	2.56	0.40
1:A:287:ARG:NH1	3:A:430:HOH:O	2.50	0.40
1:C:291:GLY:C	1:C:293:GLY:N	2.75	0.40
2:B:430:TYR:HA	2:B:431:PRO:HD3	1.92	0.40
2:B:383:ILE:N	3:B:64:HOH:O	2.55	0.40
2:B:347:ILE:N	2:B:347:ILE:HD12	2.36	0.40
2:B:378:ARG:HG2	3:B:37:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:HOH:O	3:C:461:HOH:O[4_566]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	195/198 (98%)	175 (90%)	14 (7%)	6 (3%)	5 8
1	C	193/198 (98%)	172 (89%)	14 (7%)	7 (4%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	193/239 (81%)	159 (82%)	26 (14%)	8 (4%)	3 4
All	All	581/635 (92%)	506 (87%)	54 (9%)	21 (4%)	4 6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
2	B	545	ILE
1	C	232	TRP
1	C	328	PRO
2	B	544	PRO
1	C	277	VAL
1	C	383	GLU
1	A	240	LEU
1	A	412	THR
1	A	420	ARG
2	B	331	MET
2	B	358	GLY
2	B	394	GLU
2	B	427	HIS
1	C	240	LEU
2	B	506	VAL
1	C	292	ARG
1	C	327	HIS
1	A	328	PRO
1	A	382	ALA
2	B	395	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/170 (99%)	161 (95%)	8 (5%)	32 59
1	C	167/170 (98%)	152 (91%)	15 (9%)	12 23
2	B	175/191 (92%)	161 (92%)	14 (8%)	15 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	511/531 (96%)	474 (93%)	37 (7%)	18 35

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	CYS
1	A	243	ARG
1	A	255	MET
1	A	276	ASN
1	A	288	ARG
1	A	383	GLU
1	A	396	ILE
1	A	407	LEU
2	B	316[A]	ASN
2	B	316[B]	ASN
2	B	364	LEU
2	B	366	GLN
2	B	374	GLU
2	B	378	ARG
2	B	381	LEU
2	B	396	ASP
2	B	416	ARG
2	B	424	ASP
2	B	445	ARG
2	B	449	GLN
2	B	495	LEU
2	B	545	ILE
1	C	233	CYS
1	C	242	GLN
1	C	276	ASN
1	C	297	TYR
1	C	298	TYR
1	C	299	ILE
1	C	324	TYR
1	C	327	HIS
1	C	328	PRO
1	C	385	ARG
1	C	389	VAL
1	C	398	LEU
1	C	407	LEU
1	C	418	SER
1	C	422	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	278	ASN
1	A	289	HIS
1	A	321	ASN
1	A	357	ASN
1	A	365	GLN
1	A	405	GLN
1	A	413	GLN
2	B	366	GLN
2	B	382	HIS
2	B	388	GLN
2	B	444	HIS
2	B	448	GLN
2	B	449	GLN
1	C	241	ASN
1	C	276	ASN
1	C	278	ASN
1	C	322	GLN
1	C	345	ASN
1	C	357	ASN
1	C	405	GLN
1	C	413	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	A	423	1	8,9,10	1.04	1 (12%)	8,12,14	1.87	2 (25%)
1	SEP	A	425	1	8,9,10	1.03	1 (12%)	8,12,14	2.05	3 (37%)
1	SEP	C	423	1	8,9,10	0.99	1 (12%)	8,12,14	1.85	2 (25%)
1	SEP	C	425	1	7,10,10	0.96	0	7,14,14	2.00	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	423	1	-	0/6/8/10	0/0/0/0
1	SEP	A	425	1	-	0/6/8/10	0/0/0/0
1	SEP	C	423	1	-	0/6/8/10	0/0/0/0
1	SEP	C	425	1	-	0/6/10/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	SEP	P-OG	2.20	1.67	1.60
1	C	423	SEP	P-OG	2.41	1.68	1.60
1	A	423	SEP	P-OG	2.42	1.68	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	425	SEP	O-C-CA	-2.70	118.47	125.49
1	A	423	SEP	O3P-P-O1P	-2.39	102.90	110.58
1	A	425	SEP	O3P-P-O1P	-2.30	103.17	110.58
1	C	425	SEP	O3P-P-O1P	-2.25	103.33	110.58
1	C	423	SEP	O3P-P-O1P	-2.17	103.59	110.58
1	C	425	SEP	O2P-P-O1P	2.03	117.12	110.58
1	C	425	SEP	O2P-P-OG	2.11	112.64	106.56
1	C	423	SEP	OG-P-O1P	3.03	114.85	107.14
1	C	425	SEP	OG-P-O1P	3.05	114.91	107.14
1	A	425	SEP	OG-P-O1P	3.15	115.15	107.14
1	A	423	SEP	OG-P-O1P	3.22	115.35	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	425	SEP	1	0
1	C	423	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/198 (98%)	-0.25	3 (1%) 76 71	20, 45, 93, 105	0
1	C	194/198 (97%)	-0.01	9 (4%) 36 29	31, 59, 95, 116	0
2	B	193/239 (80%)	0.59	18 (9%) 11 7	44, 77, 111, 124	0
All	All	583/635 (91%)	0.11	30 (5%) 32 25	20, 63, 104, 124	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	511	PRO	5.1
1	C	230	ALA	4.7
2	B	545	ILE	4.5
2	B	317[A]	HIS	3.9
2	B	314[A]	ILE	3.8
2	B	316[A]	ASN	3.8
1	C	325	GLY	3.8
2	B	546	ALA	3.6
2	B	318[A]	PRO	3.6
1	C	299	ILE	3.4
2	B	416	ARG	3.1
2	B	443	CYS	3.1
1	A	357	ASN	3.1
1	A	228	GLU	3.0
1	A	424	VAL	2.9
1	C	326	TRP	2.9
1	C	385	ARG	2.9
2	B	452	ALA	2.8
1	C	418	SER	2.8
2	B	453	THR	2.6
1	C	384	TYR	2.5
1	C	300	GLY	2.4
2	B	544	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	499	CYS	2.3
2	B	408	PHE	2.2
2	B	500	ILE	2.2
2	B	512	ASP	2.2
1	C	297	TYR	2.1
2	B	319[A]	ALA	2.1
2	B	399	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	425	10/11	0.89	0.12	-	99,102,104,104	0
1	SEP	A	423	10/11	0.87	0.15	-	96,99,102,103	0
1	SEP	C	423	10/11	0.96	0.12	-	51,54,60,60	0
1	SEP	C	425	11/11	0.96	0.16	-	53,62,67,67	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.